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The Crystal Structure of the Superconducting Low Temperature Phase of $C_{60}(CHCl_3)_2$ from High Resolution Powder Diffraction

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Beamline: X3B1

Introduction: Chloroform intercalated C_{60} which was first described in 1995¹ has recently drawn a lot of attention as a high T_c superconductor². Owing to the fact that single crystals do not survive during the phase transition(s) we report the structure determination of the superconducting low temperature phase from high resolution synchrotron powder diffraction data.

Methods and Materials: X-ray powder diffraction data were collected for $C_{60}(CHCl_3)_2$ at various temperatures in the range from 295 to 38 K ($\lambda = 1.15015(2)$ Å) in transmission geometry with the sample sealed in a 0.7 mm lithiumborate glass capillary (Fig. 1). Data reduction of a scan at $T = 50$ K was performed using the GUF1 program. Indexing with ITO led to a triclinic unit cell (space group P-1 with lattice parameters of $a = 9.8361(3)$, $b = 10.0905(3)$, $c = 9.8179(3)$ Å, $\alpha = 101.363(2)$, $\beta = 116.457(2)$, and $\gamma = 79.783(2)^\circ$. The crystal structure was solved using packing considerations and the GSAS Rietveld refinement package (Fig. 2). The bucky ball and the chloroform molecules were defined as rigid bodies with refinable bond lengths.

Results: $C_{60}(CHCl_3)_2$ undergoes several phase transitions upon cooling from a primitive hexagonal phase with rotationally disordered molecules towards an ordered triclinic phase. This low temperature phase can be viewed (Fig. 2) as a distorted primitive hexagonal packing of C_{60} molecules with the chloroform molecules located in the centers of the trigonal prisms. It is popularly believed that the $CHCl_3$ expands the lattice, thereby increasing the transition temperature by lowering the density of states. Our results show that the picture is more complicated, since we find two interfullerene distances significantly smaller than for pure C_{60} . Clearly the lattice symmetry and/or the fullerene orientations play a significant role in raising the transition temperature.

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References: ¹M. Jansen, G. Waidmann, Z. Anorg. Allg. Chem. 621, 14 (1995); ²J. H. Schön, Ch. Kloc, B. Batlogg, Science 293, 2432 (2001).

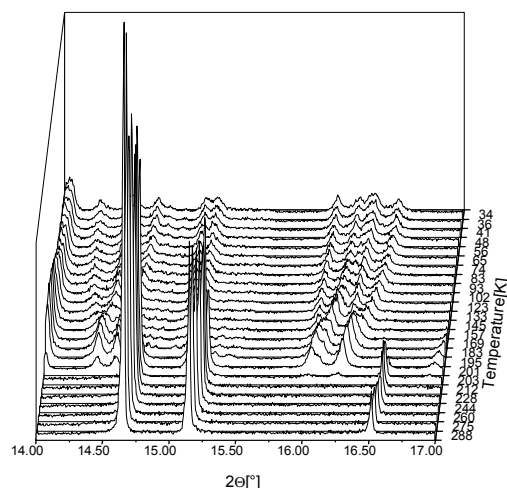


Figure 1. Scattered X-ray intensity for $C_{60}(CHCl_3)_2$ as a function of diffraction angle 2θ and temperature.

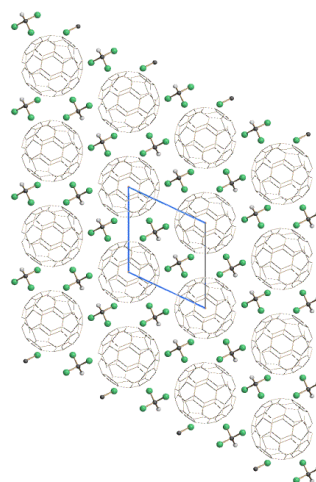


Figure 2. Ordered crystal structure of $C_{60}(CHCl_3)_2$ at $T = 50$ K in a projection along b -axis.